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DIRECT SOLUTION OF THE EQUATION OF TRANSFER USING FREQUENCY-AND--ETC(U)
JUN 79 J P APRUZESE, J DAVIS

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Direct Solution of the Equation of Transfer Using Frequency- and Angle-Averaged Photon Escape Probabilities

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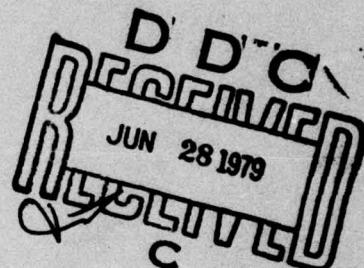
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A formalism is developed which permits direct steady-state solution of the transfer equation using escape probabilities averaged over angle and frequency. A matrix of probability-based coupling coefficients, which are related to the kernel function K_1 is used to obtain the source function for a doppler profile in plane-parallel geometry. Comparison is made with exact solutions, establishing the high accuracy of the technique. The method is extendable to different physical situations by simply modifying the coupling coefficients.

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DIRECT SOLUTION OF THE EQUATION OF TRANSFER USING FREQUENCY- AND ANGLE-AVERAGED PHOTON ESCAPE PROBABILITIES

I.   Introduction

In the literature of radiative transfer theory, much attention has been devoted to photon escape-probability concepts as a means of aiding in the interpretation of detailed solutions to the transfer equation in astrophysical and laboratory contexts. In this paper we develop a formalism which permits utilization of such concepts to <u>obtain</u> direct solutions of the steady-state source function. When applied to a plane-parallel, doppler-broadened medium, the technique eliminates entirely the need for either frequency or angle integration, while yielding generally excellent agreement with previous results obtained by Avrett and Hummer.[1]

II.   Multicell Radiative Coupling Equations

If a medium which is finite in extent in at least one direction is divided into a number N of smaller regions line photons emitted in each region will have a finite probability of being absorbed in any of the other N-1 regions, as well as being re-absorbed in the local region or escaping entirely from the medium. Let C_{ij} be the probability that a line photon emitted in geometrical region i traverses the distance between regions i and j and is absorbed in region j. N_{ui} will refer to the <u>total</u> upper level population of region i, and $A_{u\ell}$ stands for the spontaneous transition probability (sec^{-1}) for the line in question. In each region i, W_1 and D_i will stand for the total collisional population and depopulation rates, respectively, of the upper level (N_{ui}). The above concepts and notation clearly imply the following equation for the rate of change of the line upper level population in region i.

$$\frac{dN_{ui}}{dt} = N_{ei} W_i + \sum_{j=1}^{N} N_{uj} A_{u\ell} C_{ji} - N_{ui} (A_{u\ell} + D_i) \tag{1}$$

The first two terms on the right-hand-side account for local colli-
sional population of the upper level, and radiative population of the level
by photons emitted from all the cells j into cell i, respectively. The
final term is the sum of spontaneous and collisional depopulation of the
upper level. In this paper we will confine outselves to the case where
$dN_{ui}/dt = 0$, that is, utilization of equation (1) to obtain the steady
state upper level population in each region, which is equivalent to finding
the source function when the lower level population is known. For a large
class of problems, such as those treated by Avrett and Hummer[1], the
ground state (lower level) population is much larger than that of the
upper level and the absorption coefficient is known with high accuracy.
In these cases, the steady-state version of equation (1) requires for its
solution the inversion of one NxN matrix - to solve N linear equations in
N unknowns - once the C_{ji} are calculated from the absorption coefficients.
When the absorption coefficient is not known a priori, the appropriate
version of equation (1) must be set up for each level considered and
populations for each level must be obtained iteratively using the C_{ji}
calculated from the populations (hence, absorption coefficients), of the
previous iteration.

Aside from the atomic constants, calculation of the C_{ji} from the
absorption coefficients to enable solution of equation (1) forms the
heart of the mathematical problem, and is now detailed.

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III. Calculation of the Coupling Constants

For the case of plane-parallel geometry and doppler profile with a spatially constant doppler width, it has proven possible to develop very fast and extremely accurate algorithms for obtaining the C_{ji}, primarily because of the vast amount of effort by other workers which has been devoted to probability concepts for this case.

Consider a line photon emitted at a point in cell j, in the direction of cell i, in the medium. The probability P_{ji} that the photon is absorbed in cell i is given by

$$P_{ji} = \bar{P}_e(\tau_{ji}) - \bar{P}_e(\tau_{ji} + \Delta\tau_i) \tag{2}$$

where $\bar{P}_e(\tau)$ is the angle-averaged probability that a photon traverses an optical depth τ without being absorbed or scattered. In equation (2), τ_{ji} is the line-center optical depth from cell j to the boundary of cell i closest to cell j, and $\Delta\tau_i$ is the optical depth of cell i itself. The practicality of the method here described is obviously dependent upon having an efficient technique for obtaining the $\bar{P}_e$'s. Holstein[2] obtained an expression for the monodirectional escape probability P_e valid for completely redistributed doppler-profile line photons at large optical depths. We have numerically calculated the integral

$$\bar{P}_e(\tau_0) = \int_0^1 P_e\left(\frac{\tau_0}{\mu}\right) d\mu \tag{3}$$

for a large range of optical depths, and have adopted the following algorithm to obtain $\bar{P}_e$ quickly and accurately.

(a.) at $\tau_0 \leq 3$ a cubic spline polynomial has been fitted to the exact result at 20 points roughly equally spaced from $\tau_0 = 0$ to $\tau_0 = 3$.

(b) for $\tau_0 > 3$; the following analytic expression is accurate to
5 percent for $\tau < 3 \times 10^4$.

$$\overline{P}_e \ (\tau_0) = \frac{0.286}{\tau_0 \ \sqrt{\ln \ (1.95 \ \tau_0)}}$$

At this point it should be noted that in calculating the C_{ji} coupling
cells of finite width, $\overline{P}_e$ must be averaged over the cell originating
the photons. This is especially important when the originating and
receiving cells are adjacent, since $\overline{P}_e$ can vary by an order of magnitude
or more, in some cases, from the front to the back of the originating cell.
This averaging process is easily accomplished by analytically integrating
the above expressions across the originating cell j so that

$$C_{ji} = \frac{1}{2(\Delta\tau)_j} \left\{ \int_{\tau_{ji}}^{\tau_{ji} + \Delta\tau_j} \overline{P}_e(\tau)d\tau - \int_{\tau_{ji} + \Delta\tau_i}^{\tau_{ji} + (\Delta\tau)_i + (\Delta\tau)_j} \overline{P}_e(\tau)d\tau \right\} \qquad (4)$$

In equation (4), $(\Delta\tau)_j$ and $(\Delta\tau)_i$ are the line-center perpendicular optical
depths of cells j and i and τ_{ji} is the optical depth between cells j and
i, measured between the two closest boundaries. The factor of 1/2 in
equation (4) accounts for the assumed equal probability of photon emission
in either direction from cell j.

IV.   Relation to the Exact Transfer Equation

Avrett and Hummer[1] have written the formal solution for the source
function $S(\tau)$ in a plane-parallel atmosphere of optical depth T as

$$S(\tau) = (1-P_Q) \int_0^T K_1(|t-\tau|) \ S(t)dt \ + \ P_Q B \qquad (5)$$

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where B is the Planck function for the local electron temperature, P_Q is the "quenching parameter", or probability per scattering that the photon is lost from the line, and K_1 is the kernel function. In reference 1, Avrett and Hummer developed a useful asymptotic expansion for the Doppler kernel function and showed that, for large τ (measured at line center)

$$K_1(\tau) \sim \frac{1}{4\pi\tau^2\sqrt{\ln\tau}} \tag{6}$$

Inspection of equation (5) reveals that $K_1(\tau)$ is the analog of the discrete probability-based coupling coefficients which are used in the present treatment. $K_1(\tau)$ couples the regions of the medium together and, since the integral is carried out over τ, it is, in analogy with equations (1) and (2)

$$K_1(\tau_o) = -\frac{1}{2}\frac{d\overline{P}_e}{d\tau}\bigg|_{\tau_o} \tag{7}$$

The rate of change of the angle-averaged escape probability $\overline{P}_e$ across optical path τ_o determines the efficiency with which photons are absorbed per unit optical depth after crossing the path τ_o.

The analytic expression

$$\overline{P}_e(\tau_o) = 0.286 / \tau_o \sqrt{\ln(1.95\tau_o)} \tag{8}$$

which we have used computationally in the calculations presented below should, when differentiated, approach closely equation (7) in the limit of large τ.

Differentiating equation 8 yields, as $\tau \to \infty$

$$-\frac{1}{2}\frac{d\overline{P}_e}{d\tau}_{\tau \to \infty} = \frac{1}{13.99\ \tau^2\sqrt{\ln\tau}} \tag{9}$$

(τ measured at line center)

which differs by 11% from the exact expression (6.). Even though our expression is not as accurate at $\tau = \infty$ as at $\tau < 3 \times 10^{+4}$, no divergence occurs. For most cases of interest, nearly all of the coupling occurs within optical depths much smaller than 3×10^4, where equation (8) is accurate to better than 5%. Also, as seen below, errors of a few percent in the coupling matrix do not result in large source function errors when the method is applied to specific media of finite optical depth.

V.   Calculations and Discussion

a) Numerical Results

To explore the computational viability of the approach detailed above, we have applied equation (1) to a range of plane-parallel media of varying optical depths and quenching parameters. The cases presented in figures 1 and 2 reflect comparisons of the presently discussed approach with exact solutions obtained by Avrett and Hummer[1]. The physical interpretation of the solutions has been thoroughly discussed in reference 1 by Avrett and Hummer. Since the media are symmetric about the midplane, the calculation has been set up by establishing 25 or 75 cells in half the medium and coupling each cell "to itself" and to others across the symmetry plane as well as by direct photon coupling within the same half of the medium. In each case the cells are spaced logarithmically in optical depth ($\Delta \tau / \tau \sim$ constant) and the optical depths of the cells close to the boundary are less than unity to allow for the anticipated rapid change of the source function near the edge of the medium. We have also computed results for 50 cells per half-slab, which are not plotted for reasons of clarity.

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To obtain solutions within a few percent of the exact values, only 25 cells need be used for optical depths of $\sim 10^2$, but 50-75 cells are necessary at $\tau \sim 10^4$. These considerations apply for both the effectively thick and the effectively thin cases. As is seen in figure 2, for $\tau = 2.8 \times 10^7$, the 25-cell calculation yields source functions a factor of 2.5 greater than the exact solution at small optical depths, but goes to the Planck function (B = 1) at the correct optical depth. The 75-cell model yields source functions about 25% too high in the nonthermalized "effectively thin" regions at this very high optical depth.

b) Applications and Discussion

The technique described above appears to hold considerable promise for computationally efficient modeling of laboratory plasmas. Detailed multi-angle, multi-frequency calculations have shown[3] that the ionization dynamics and energetics of high-temperature plasmas are significantly affected by the trapping of line and continuum radiation. Accurate simulation of such plasmas and computation of diagnostically useful line ratios requires that all optically thick lines be transported. The elimination of angle- and frequency-integrations inherent in this technique can lead to both accurate and rapid computation of detailed radiation transport in plasma simulations such as those described in reference 3. Extending the usefulness of the method will require attention to obtaining accurate coupling coefficients including the effects of continuum processes, Voigt profiles (whose width may vary temporally and spatially), and non-planar geometry. The numerical consequences of this additional physics will appear solely in the use of different coupling coefficients. Work on obtaining efficient algorithms for the calculation of such

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coefficients is proceeding, and will be reported in later papers. In
addition, other transitions will be incorporated to study multi-level,
multi-ionization-stage effects.

ACKNOWLEDGMENT

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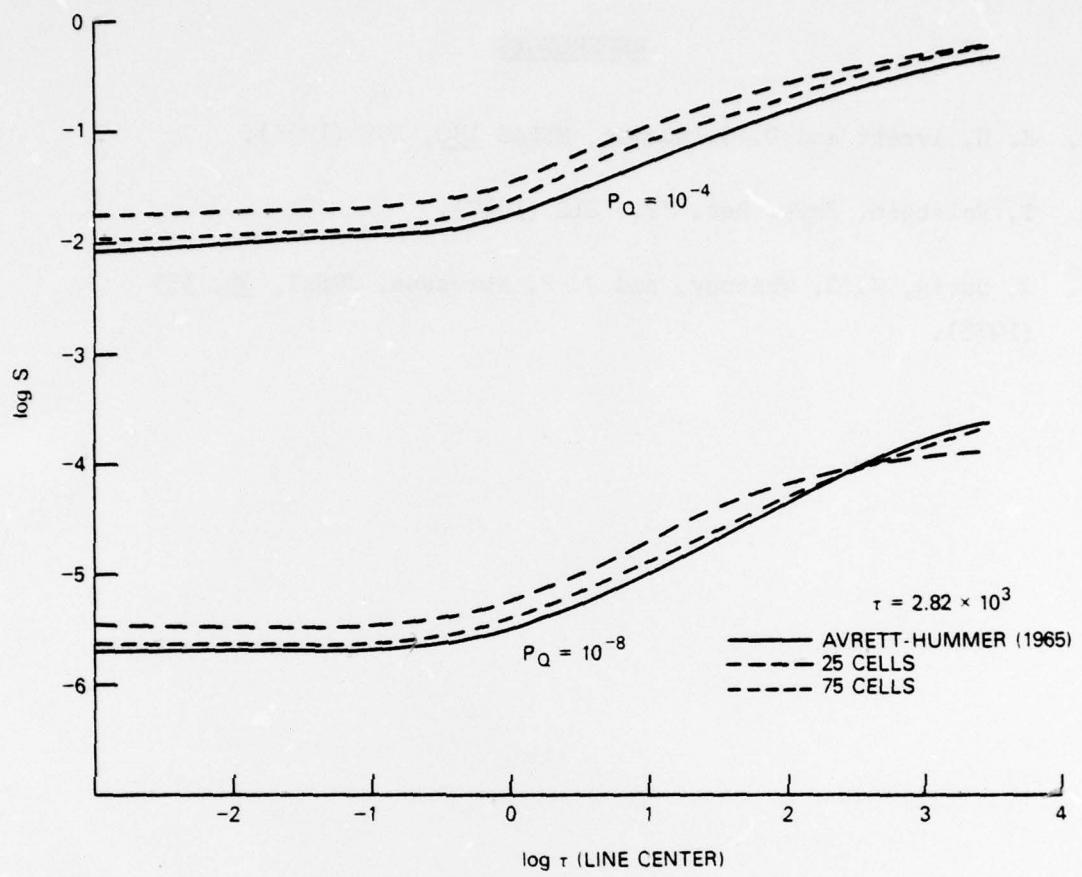
Fig. 1

The steady state source function for a doppler profile is
shown for an optical depth of 2.82×10^{3} and a Planck
function $B = 1$. Results obtained from the present treatment
are shown along with the exact solutions obtained by Avrett
and Hummer in Ref. 1. The optical depth is measured from
the center of the plane - parallel medium to the edge
and at line center. Quenching parameters of 10^{-4} (effec-
tively thick) and 10^{-8} (effectively thin) are assumed in
the curves shown.

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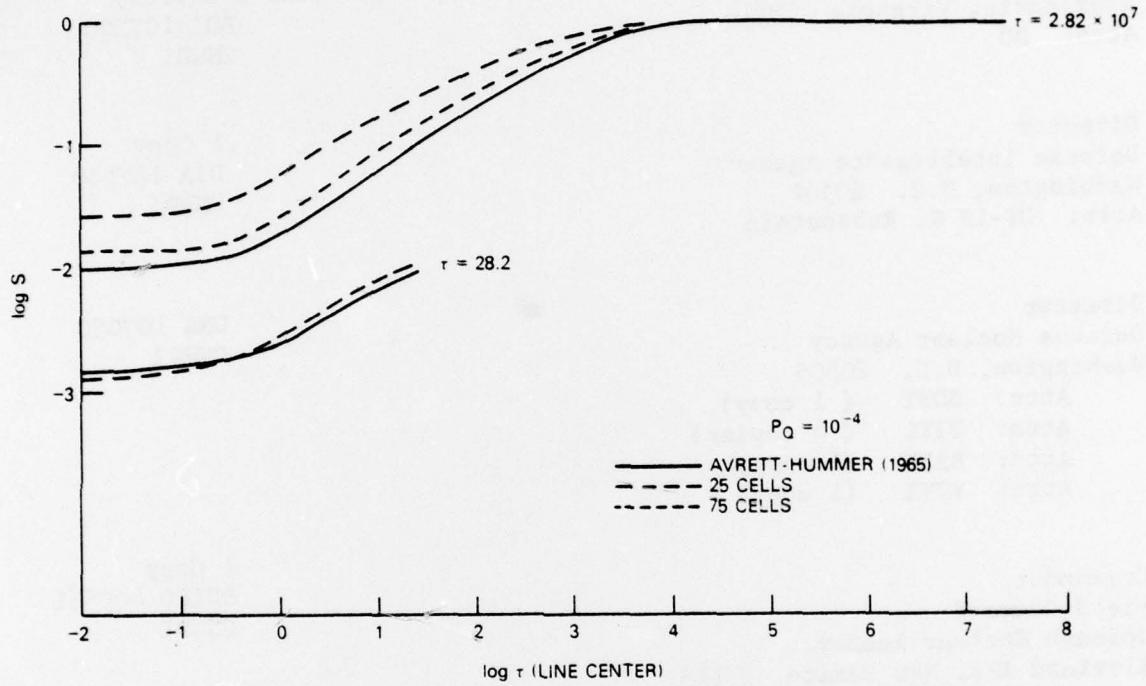
Fig. 2

Same as Figure 1, except that optical depths of 28.2 and
2.82×10^7 are shown, and only one quenching parameter,
10^{-4}, is considered.

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